

=> fil reg

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STRUCTURE FILE UPDATES: 12 NOV 94 HIGHEST RN 158930-02-0
DICTIONARY FILE UPDATES: 14 NOV 94 HIGHEST RN 158930-02-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

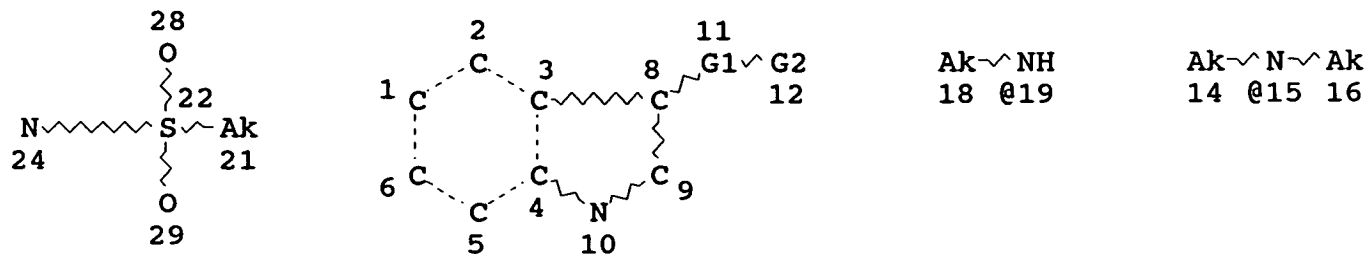
=>

=>

=> d que 15

L3

STR



REP G1=(1-4) C

VAR G2=NH2/15/19

NODE ATTRIBUTES:

NSPEC IS R AT 24

CONNECT IS E1 RC AT 14

CONNECT IS E1 RC AT 16

CONNECT IS E1 RC AT 18

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L5 22 SEA FILE=REGISTRY SSS FUL L3

=> d 15 1-22 ide can

L5 ANSWER 1 OF 22 REGISTRY COPYRIGHT 1994 ACS

RN 157694-77-4 REGISTRY

CN Piperazine, 1-[[[3-(2-aminoethyl)-1H-indol-5-yl]oxy]methyl]sulfonyl]-4-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

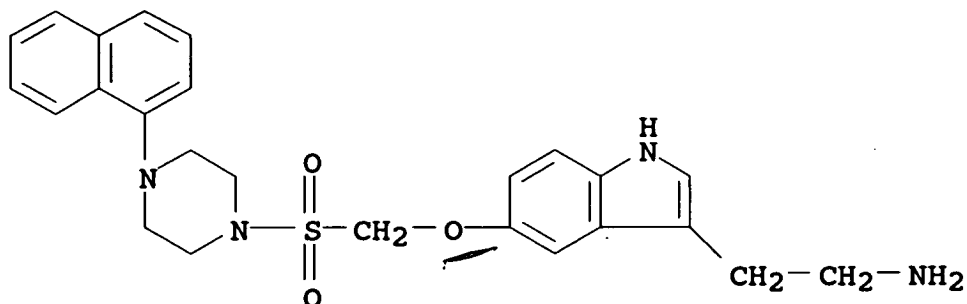
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MF C25 H28 N4 O3 S

CI COM

SR CA

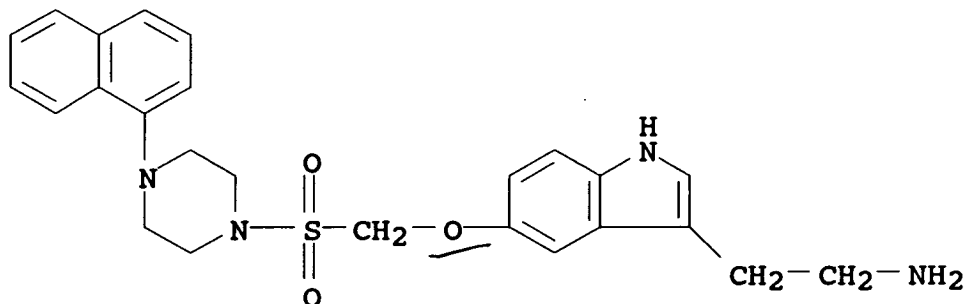
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:179613

L5 ANSWER 2 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 157694-76-3 REGISTRY
CN Piperazine, 1-[[[3-(2-aminoethyl)-1H-indol-5-yl]oxy]methyl]sulfonyl]-4-(1-naphthalenyl)-, hydrochloride (9CI)
(CA INDEX NAME)
MF C25 H28 N4 O3 S . x Cl H
SR CA
LC STN Files: CA
CRN (157694-77-4)

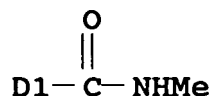
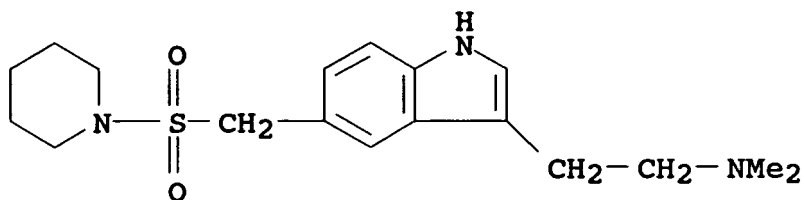


●x HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 121:179613

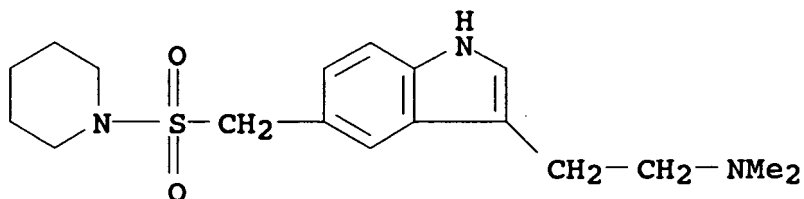
L5 ANSWER 3 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154360-36-8 REGISTRY
CN Piperidinecarboxamide, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-N-methyl- (9CI) (CA INDEX NAME)
MF C20 H30 N4 O3 S
CI IDS
SR CA
LC STN Files: CA
DES 8:ID,RING(C5N1)



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

L5 ANSWER 4 OF 22 REGISTRY COPYRIGHT 1994 ACS
 RN 154360-35-7 REGISTRY
 CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl](phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)
 MF C25 H33 N3 O2 S . Cl H
 CI IDS
 SR CA
 LC STN Files: CA
 DES 8:ID,RING(C5N1)



● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

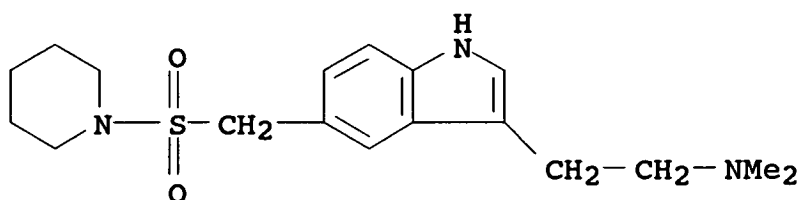
L5 ANSWER 5 OF 22 REGISTRY COPYRIGHT 1994 ACS
 RN 154360-34-6 REGISTRY
 CN Butanedioic acid, compd. with 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]methoxypiperidine (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]methoxy-, butanedioate (1:1) (9CI)
MF C19 H29 N3 O3 S . C4 H6 O4
SR CA
LC STN Files: CA

CM 1

CRN 154360-33-5
CMF C19 H29 N3 O3 S
CCI IDS
CDES 8:ID,RING(C5N1)



D1-O-Me

CM 2

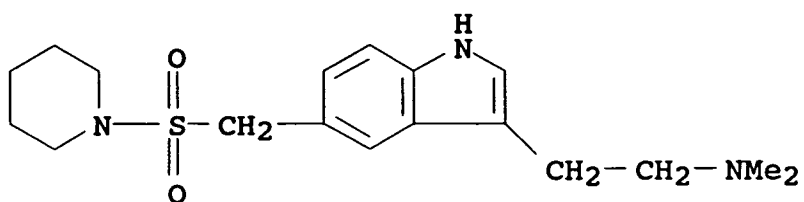
CRN 110-15-6
CMF C4 H6 O4

HO₂C-CH₂-CH₂-CO₂H

1 REFERENCES IN FILE CA (1967 TO DATE)

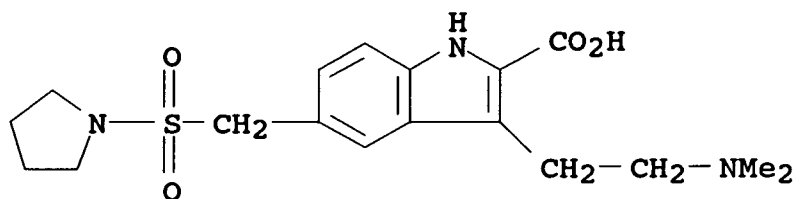
REFERENCE 1: P 120:244669

L5 ANSWER 6 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154360-33-5 REGISTRY
CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]methoxy- (9CI) (CA INDEX NAME)
MF C19 H29 N3 O3 S
CI IDS, COM
SR CA
DES 8:ID,RING(C5N1)



D1-O-Me

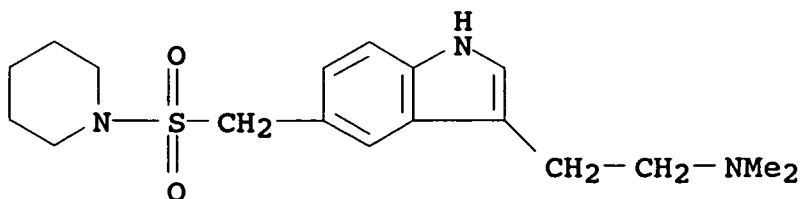
L5 ANSWER 7 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-59-8 REGISTRY
CN 1H-Indole-2-carboxylic acid, 3-[2-(dimethylamino)ethyl]-5-[(1-pyrrolidinylsulfonyl)methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H25 N3 O4 S
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

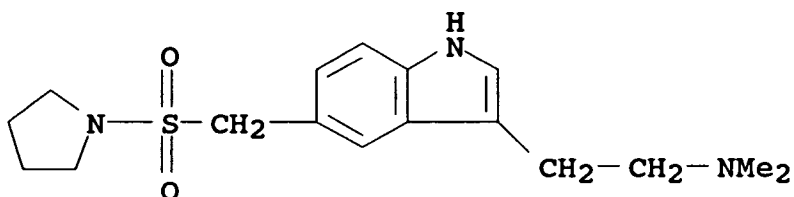
L5 ANSWER 8 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-58-7 REGISTRY
CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H27 N3 O2 S
CI COM
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

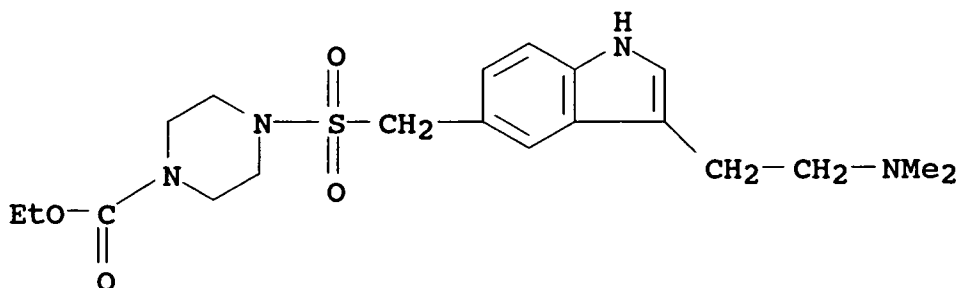
L5 ANSWER 9 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-57-6 REGISTRY
CN Pyrrolidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H25 N3 O2 S
CI COM
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

L5 ANSWER 10 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-56-5 REGISTRY
CN 1-Piperazinecarboxylic acid, 4-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H30 N4 O4 S
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

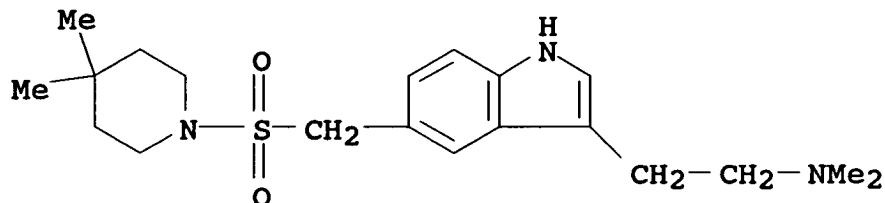
REFERENCE 1: P 120:244669

L5 ANSWER 11 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-55-4 REGISTRY
CN Butanedioic acid, compd. with 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-4,4-dimethylpiperidine (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-

yl]methyl]sulfonyl]-4,4-dimethyl-, butanedioate (1:1) (9CI)
MF C20 H31 N3 O2 S . C4 H6 O4
SR CA
LC STN Files: CA

CM 1

CRN 154323-54-3
CMF C20 H31 N3 O2 S



CM 2

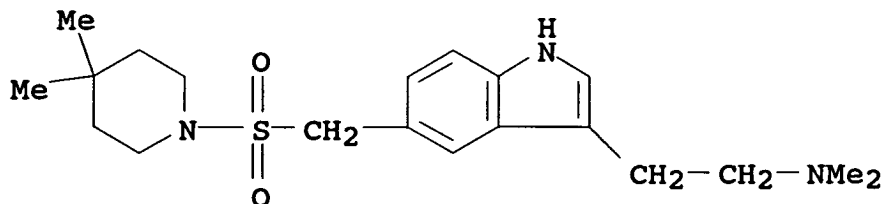
CRN 110-15-6
CMF C4 H6 O4



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

L5 ANSWER 12 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-54-3 REGISTRY
CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-4,4-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H31 N3 O2 S
CI COM
SR CA



L5 ANSWER 13 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-53-2 REGISTRY
CN Butanedioic acid, compd. with 1-[[[3-[2-(dimethylamino)ethyl]-1H-

indol-5-yl)methylsulfonyl]-4-methylpiperidine (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl)methylsulfonyl]-4-methyl-, butanedioate (1:1) (9CI)

MF C19 H29 N3 O2 S . C4 H6 O4

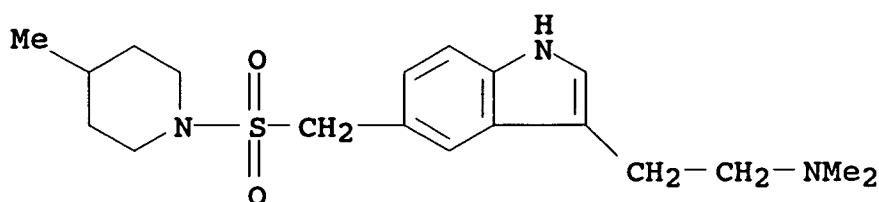
SR CA

LC STN Files: CA

CM 1

CRN 154323-52-1

CMF C19 H29 N3 O2 S



CM 2

CRN 110-15-6

CMF C4 H6 O4

HO₂C-CH₂-CH₂-CO₂H

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

L5 ANSWER 14 OF 22 REGISTRY COPYRIGHT 1994 ACS

RN 154323-52-1 REGISTRY

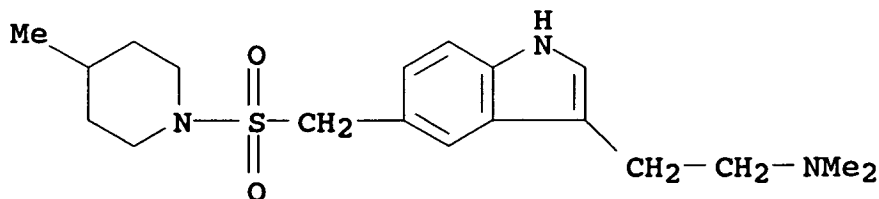
CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl)methylsulfonyl]-4-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H29 N3 O2 S

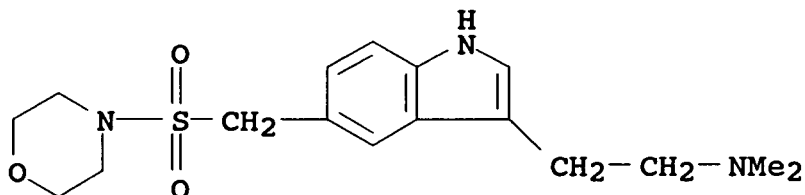
CI COM

SR CA



L5 ANSWER 15 OF 22 REGISTRY COPYRIGHT 1994 ACS

RN 154323-51-0 REGISTRY
CN Morpholine, 4-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)
MF C17 H25 N3 O3 S . Cl H
SR CA
LC STN Files: CA

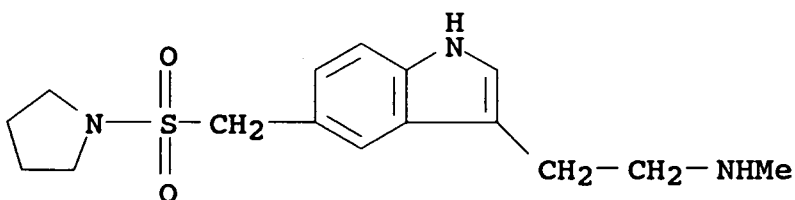


● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

L5 ANSWER 16 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-50-9 REGISTRY
CN Pyrrolidine, 1-[[[3-[2-(methylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)
MF C16 H23 N3 O2 S . Cl H
SR CA
LC STN Files: CA



● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

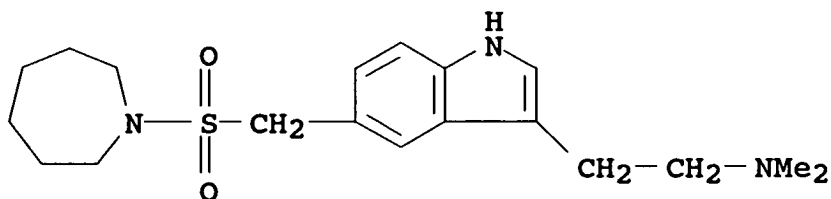
REFERENCE 1: P 120:244669

L5 ANSWER 17 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-49-6 REGISTRY
CN Butanedioic acid, compd. with 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]hexahydro-1H-azepine (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:

CN 1H-Azepine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]hexahydro-, butanedioate (1:1) (9CI)
MF C19 H29 N3 O2 S . C4 H6 O4
SR CA
LC STN Files: CA

CM 1

CRN 154323-48-5
CMF C19 H29 N3 O2 S



CM 2

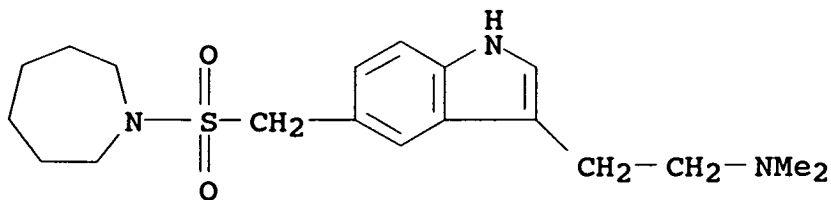
CRN 110-15-6
CMF C4 H6 O4

HO₂C-CH₂-CH₂-CO₂H

1 REFERENCES IN FILE CA (1967 TO DATE)

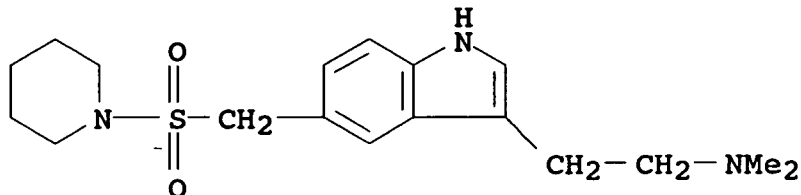
REFERENCE 1: P 120:244669

L5 ANSWER 18 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-48-5 REGISTRY
CN 1H-Azepine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]hexahydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H29 N3 O2 S
CI COM
SR CA



L5 ANSWER 19 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-47-4 REGISTRY
CN Piperidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

MF C18 H27 N3 O2 S . Cl H
SR CA
LC STN Files: CA
CRN (154323-58-7)

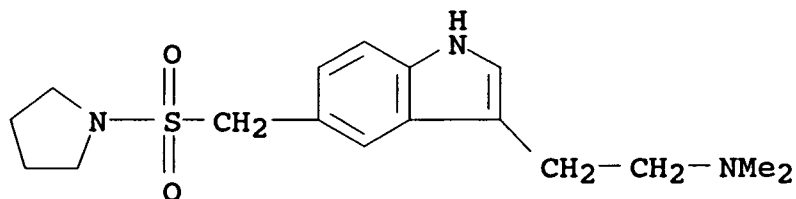


● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

L5 ANSWER 20 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 154323-46-3 REGISTRY
CN Pyrrolidine, 1-[[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)
MF C17 H25 N3 O2 S . Cl H
SR CA
LC STN Files: CA
CRN (154323-57-6)



● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:244669

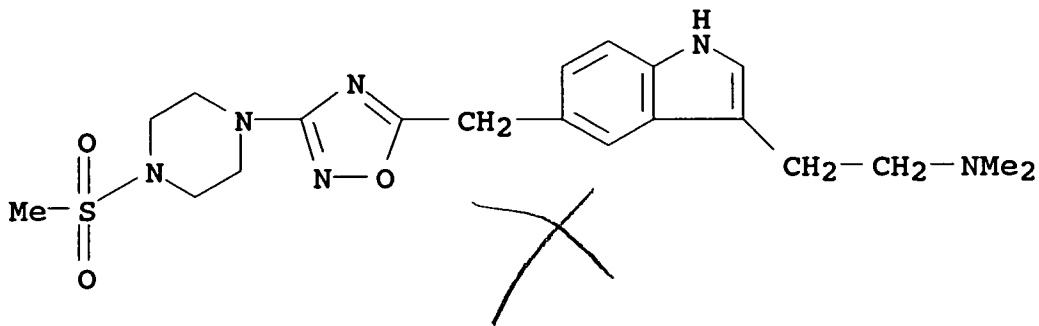
L5 ANSWER 21 OF 22 REGISTRY COPYRIGHT 1994 ACS
RN 137404-32-1 REGISTRY
CN Piperazine, 1-[5-[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]-1,2,4-oxadiazol-3-yl]-4-(methylsulfonyl)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)
MF C20 H28 N6 O3 S . C2 H2 O4
SR CA

LC STN Files: CA

CM 1

CRN 137404-31-0

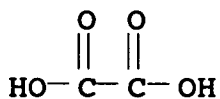
CMF C20 H28 N6 O3 S



CM 2

CRN 144-62-7

CMF C2 H2 O4



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 116:83677

L5 ANSWER 22 OF 22 REGISTRY COPYRIGHT 1994 ACS

RN 137404-31-0 REGISTRY

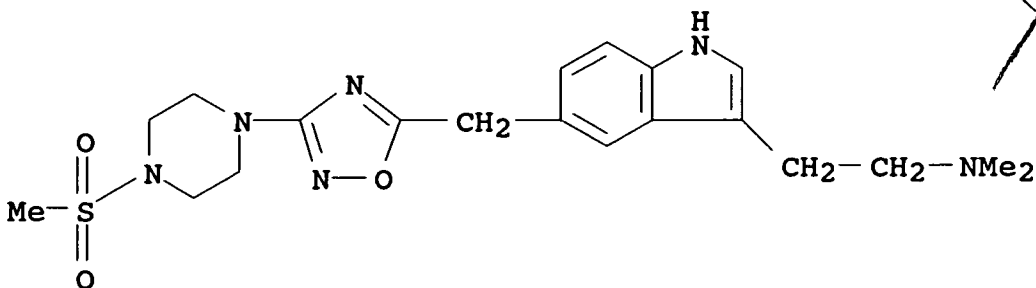
CN Piperazine, 1-[5-[[3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]methyl]-1,2,4-oxadiazol-3-yl]-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H28 N6 O3 S

CI COM

SR CA



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FILE 'CA' ENTERED AT 08:47:34 ON 15 NOV 94
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FILE COVERS 1967 - 12 Nov 1994 (941112/ED) VOL 121 ISS 20

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SmartSELECT searches with large numbers of terms.

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(FILE 'WPIDS' ENTERED AT 08:14:21 ON 15 NOV 94)
DEL HIS Y

FILE 'REGISTRY' ENTERED AT 08:37:50 ON 15 NOV 94

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L2 0 S L1
L3 STR L1
L4 0 S L3
L5 22 S L3 FUL

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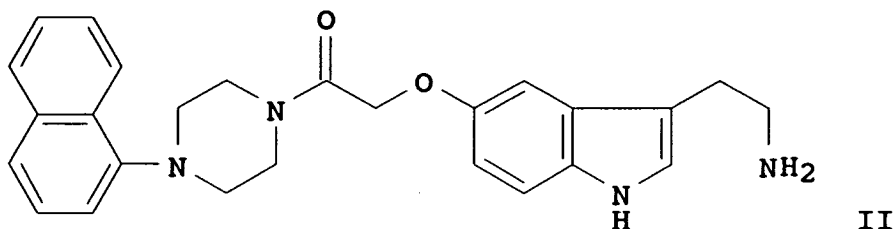
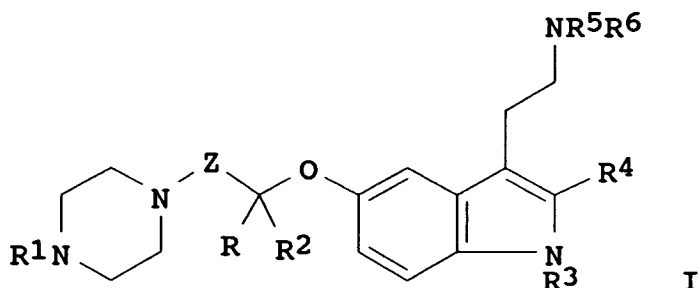
L6 3 S L5

FILE 'REGISTRY' ENTERED AT 08:45:59 ON 15 NOV 94

FILE 'CA' ENTERED AT 08:47:34 ON 15 NOV 94

=> d 1-3 bib abs hitrn

L6 ANSWER 1 OF 3 CA COPYRIGHT 1994 ACS *cite!* *too new*
AN 121:179613 CA
TI Preparation of 5-[(piperazinocarbonyl)methoxy]tryptamines and
analogs as 5-HT receptor ligands
IN Halazy, Serge; Perez, Michel; Briley, Michael
PA Pierre Fabre Medicament, Fr.
SO Fr. Demande, 53 pp.
CODEN: FRXXBL
PI FR 2699918 A1 940701 *LATE*
AI FR 92-15919 921230
DT Patent
LA French
OS MARPAT 121:179613
GI



AB Title compds [I; R = H, alkyl, Ph; R1 = H, (cyclo)alkyl, Ph, CH2Ph, naphthyl, etc.; R2 = H, (cyclo)alkyl, Ph, CH2Ph, pyrrolyl, pyridyl, etc.; R3, R5 = H, alkyl, CH2Ph, CH2CH2Ph; R4 = H, Cl, F, Br, alkyl; R6 = H, alkyl, COR7, CO2R7, CONHR7; R7 = alkyl, (un)substituted Ph; Z = CO, SO2, (CH2)1-5] were prepd. Thus, N-(1-naphthyl)piperazine was condensed with ClCH2COCl and the product condensed with N-BOC-5-hydroxytryptamine to give, after deprotection, title compd. II which had IC50 of 115x10-9M and 3.2x10-9M against 5-HT binding at 5-HT1A and 5-HT1D receptors of sheep caudate nucleus prepn. in vitro, resp.

IT 157694-76-3P 157694-77-4P
(prepn. of, as 5-HT receptor ligand)

L6 ANSWER 2 OF 3 CA COPYRIGHT 1994 ACS

AN 120:244669 CA

TI Preparation of [3-(2-aminoethyl)-5-indolyl]methanesulfonamides as antimigraine agents

IN Fernandez Forner, Dolores; Puig Duran, Carles; Prieto Soto, Jose; Vega Noverola, Armando; Moragues Mauri, Jacinto

PA Laboratorios Almirall S.A., Spain

SO PCT Int. Appl., 21 pp.

CODEN: PIXXD2

PI WO 9402460 A1 940203

DS W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN

RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 93-EP1901 930719

PRAI GB 92-16009 920728

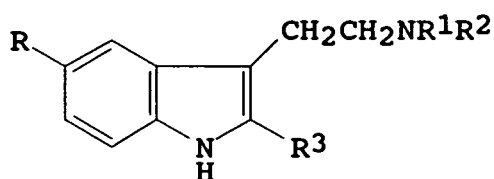
DT Patent

LA English

OS MARPAT 120:244669

GI

APP'S PCT



I

AB Title compds. (I; R = CH₂SO₂Z) [II; R₁, R₂ = H, alkyl; R₃ = H; Z = morpholino, (substituted)piperidino, pyrrolidino, 4-(alkoxycarbonyl)piperazino, etc.] were prepd. Thus, II (R₁ = R₂ = Me, Z = pyrrolidino) (III; R₃ = CO₂H) was decarboxylated to give III (R₃ = H) which had IC₅₀ of 10.4 and 460nM against ligand binding at 5-HT_{1D} and 5-HT_{1A} receptors in vitro, resp.

IT 154323-46-3P 154323-47-4P 154323-49-6P

154323-50-9P 154323-51-0P 154323-53-2P

154323-55-4P 154323-56-5P 154323-57-6P

154323-58-7P 154360-34-6P 154360-35-7P

154360-36-8P

(prepn. of, as antimigraine agent)

IT 154323-59-8

(reaction of, in prepn. of antimigraine agent)

L6 ANSWER 3 OF 3 CA COPYRIGHT 1994 ACS

AN 116:83677 CA

TI Preparation of substituted (1,2,4-oxadiazolyldindolyl)ethylamine and analogs as agonists of 5-HT₁-like receptors

IN Baker, Raymond; Reeve, Austin J.; Street, Leslie J.

PA Merck Sharp and Dohme Ltd., UK

SO Eur. Pat. Appl., 58 pp.

CODEN: EPXXDW

PI EP 438230 A2 910724

DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

AI EP 91-300180 910110

PRAI GB 90-1018 900117

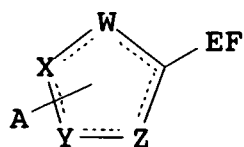
GB 90-8587 900417

DT Patent

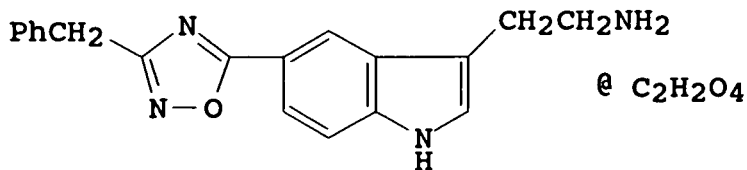
LA English

OS MARPAT 116:83677

GI



I



IV

AB Title compds. I [wherein the broken circle represents 2 non-adjacent double bonds in any position; W, X, Y, Z = O, S, N, C, such that 1 of W, X, Y, Z = O, S and at least 1 of W, X, Y, Z = C; A = H, hydrocarbyl, halo, NC, F₃C, O₂N, etc.; E = bond, C1-4 alkylene, F =

(substituted) heterocyclyl] or a salt or prodrug thereof, are prepd. NaNO₂ was added to 4-(H₂N)C₆H₄CO₂Et in concd. HCl, the mixt. stirred at 0.degree. before adding SnCl₂.2H₂O in HCl to give 4-(H₂NNH)C₆H₄CO₂Et.HCl (II). II and 4-ClCH₂(CH₂)₂CH(OMe)₂ in EtOH/H₂O were refluxed, the solvent removed and the residue chromatographed to give 2-(5-5-carbethoxy-1H-indol-3-yl)ethylamine.H maleate (III). NaH was added to phenylacetamide oxime in THF, the reaction mixt. refluxed, III was added and the whole refluxed for 2 h, the reaction mixt. cooled to room temp. to give the title compd. as the H.oxalate (IV). The activity as agonist of 5-HT₁-like receptor was measured in terms of their ability to mediate contraction of the saphenous vein of rabbits, and the potency calcd. as -log₁₀EC₅₀ (pEC₅₀). The pEC₅₀ of IV was not less than 5.0. Tablet compns. comprising I are given.

IT 137404-32-1P

(prepn. of, as 5-HT₁ agonists)

=> fil caold caprev

FILE 'CAOLD' ENTERED AT 08:48:17 ON 15 NOV 94

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=> s 15

FILE 'CAOLD'

L7 0 L5

FILE 'CAPREVIEWS'

L8 0 L5

TOTAL FOR ALL FILES

L9 0 L5

=> fil reg

FILE 'REGISTRY' ENTERED AT 08:48:32 ON 15 NOV 94

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DICTIONARY FILE UPDATES: 14 NOV 94 HIGHEST RN 158930-02-0

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

=> fil casrea

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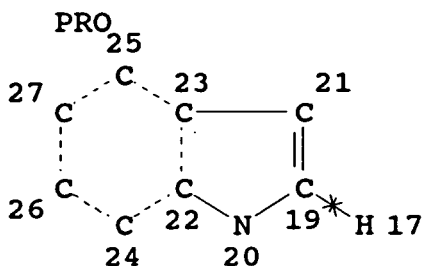
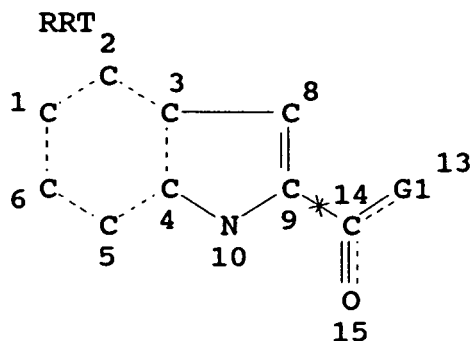
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FILE CONTENT: 1985-1994 (VOL 102 ISS 1 - VOL 121 ISS 17)

>>> Several important enhancements to CASREACT functional group <<<
>>> searching were introduced. Enter HELP FGA or HELP FGC for more <<<
>>> information. <<<

=> d que 15

L1 STR



VAR G1=OH/OME

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

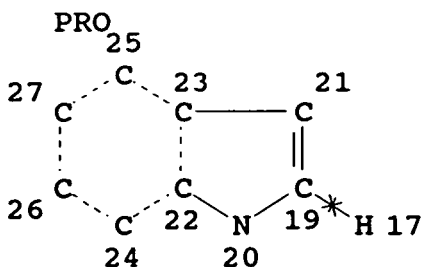
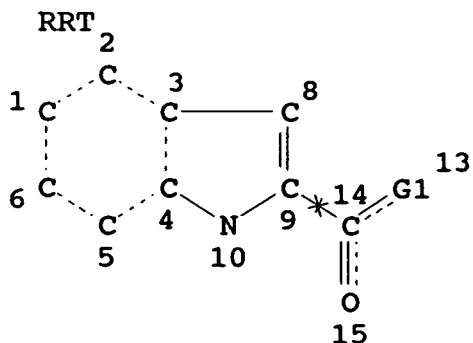
STEREO ATTRIBUTES: NONE

****MAPPINGS****

NOD	SYM	ROL	NOD	SYM	ROL
9	C	RRT	19	C	PRO
10	N	RRT	20	N	PRO
19	C	PRO	9	C	RRT
20	N	PRO	10	N	RRT

L3 29 SEA FILE=CASREACT SSS FUL L1 (73 REACTIONS)

L4 STR



Subset Search to
Narrow

VAR G1=OH/OME
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

****MAPPINGS****

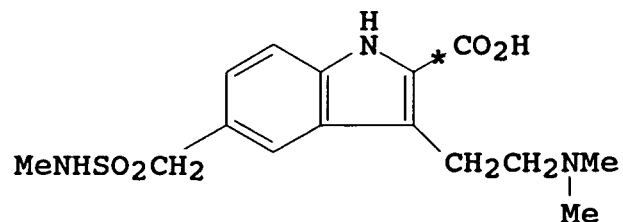
NOD	SYM	ROL	NOD	SYM	ROL
9	C	RRT	19	C	PRO
10	N	RRT	20	N	PRO
19	C	PRO	9	C	RRT
20	N	PRO	10	N	RRT

L5 17 SEA FILE=CASREACT SUB=L3. SSS FUL L4 (40 REACTIONS)

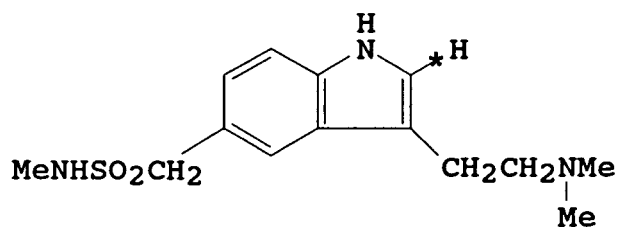
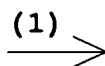
=> d l5 1-17 fhlt bib abs

L5 ANSWER 1 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(1) OF 2 A ==> B



A



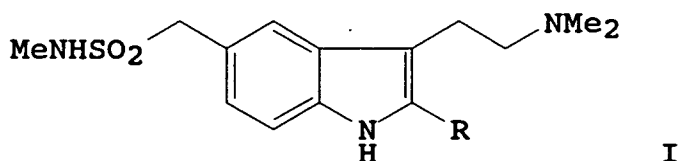
B

YIELD 80%

RX(1) RCT A 153654-26-3
PRO B 103628-46-2
CAT 1317-39-1 Cu2O
SOL 91-22-5 Quinoline

NTE N atm., evolution of CO₂, 205.degree.

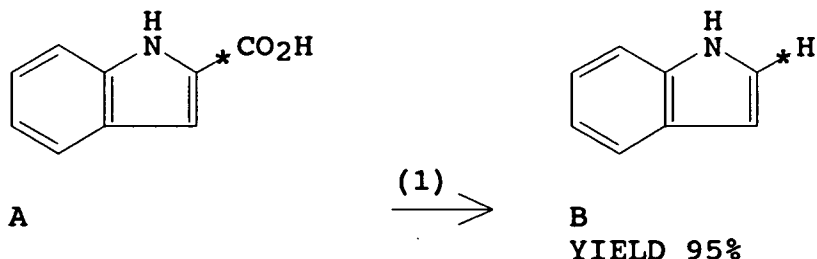
AN 120:191533 CASREACT
 TI Process for the preparation of 3-[2-(dimethylamino)ethyl]-N-methyl-1H-indole-5-methanesulfonamide [sumatriptan]
 IN Dalmases Barjoan, Pere; Marquillas Olondriz, Francisco; Bosch Rovira, Anna; Caldero Ges, Jose Maria
 PA Inke, S.A., Spain
 SO Span., 4 pp.
 CODEN: SPXXAD
 PI ES 2033578 A1 930316
 AI ES 91-1360 910606
 DT Patent
 LA Spanish
 GI



AB The title compd. I (R = H) (II), useful for the treatment of migraine (no data), is prepd. by catalytic decarboxylation of the carboxylic acid I (R = CO₂H) (III) in a solvent medium. Thus, heating of III with Cu₂O in dry quinoline under N at 205.degree. for 30-40 min gave 80% II. Similar reaction using powd. Cu catalyst in a mixt. of quinoline and di-Ph ether over 1 h gave 69% II. II was also converted to its 1:1 succinate salt.

L5 ANSWER 2 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(1) OF 5 A ==> B



RX(1) RCT A 1477-50-5
 PRO B 120-72-9
 SOL 91-22-5 Quinoline
 NTE microwave

AN 119:180622 CASREACT
 TI Decarboxylation of indole-2-carboxylic acids: improved procedures
 AU Jones, Graham B.; Chapman, Brant J.
 CS Dep. Chem., Clemson Univ., Clemson, SC, 29634-1905, USA
 SO J. Org. Chem. (1993), 58(20), 5558-9

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

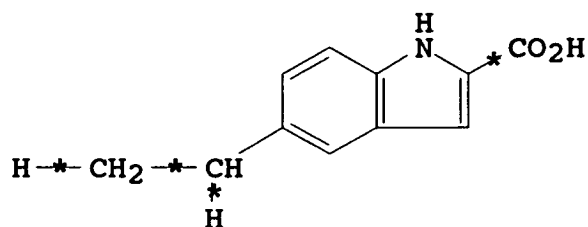
LA English

OS CJACS-IMAGE; CJACS

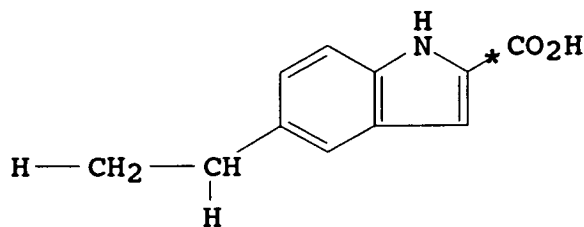
AB The microwave induced decarboxylation of a variety of indole-2-carboxylates has been studied and accomplished. Optimal yields for decarboxylation were obtained either by conducting the thermolyses in the absence of a solvent or in quinoline soln. Yields were comparable either in the absence of a catalyst or using a catalytic amt. of either copper powder or copper (I) chloride. The copper(II) salt of indole-2-carboxylic acid, which undergoes in situ redn. to the copper(I) species was also found to be effective. Near quant. yields of decarboxylated indoles were recovered following a 12 min microwave thermolysis at 600w using a com. oven. Both methoxy and fluoro substituted indoles are amenable to the process, which is conducted in a sealed tube for best results.

L5 ANSWER 3 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(1) OF 1 2 A ==> B + C

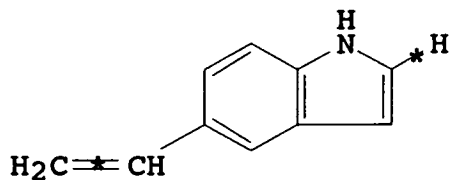


A

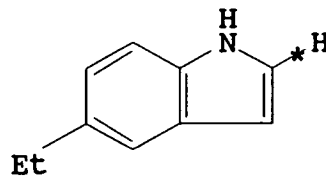


A

(1) →



B
YIELD 26%



C
YIELD 14%

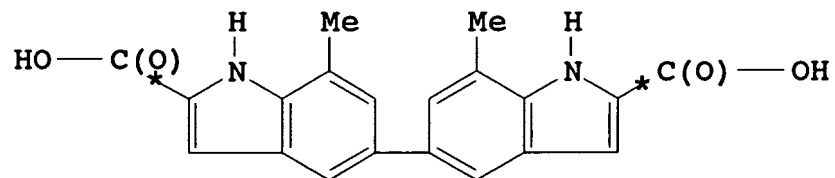
RX(1) RCT A 37033-93-5
PRO B 77132-99-1, C 68742-28-9
CAT 39320-55-3 K 16 (catalyst)
SOL 71-43-2 Benzene

AN 115:232027 CASREACT

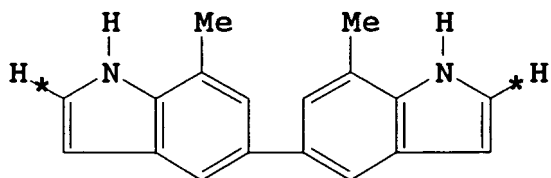
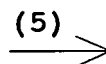
TI The synthesis of 5-vinylindole by simultaneous dehydrogenation and decarboxylation of 5-ethylindole-2-carboxylic acid and its ethyl ester

AU Starostenko, N. E.; Phung Tien Dat; Serova, I. A.; Kamenetskii, A. V.; Suvorov, N. N.
CS Mosk. Khim.-Tekhnol. Inst., Moscow, 125047, USSR
SO Khim. Geterotsikl. Soedin. (1991), (5), 638-41
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
AB A new method of prepn. of 5-vinylindole by catalytic dehydrogenation/decarboxylation of 5-ethylindolecarboxylic acid or its Et ester over a K-16 catalyst is presented.
L5 ANSWER 4 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(5) OF 15 ...M ==> O

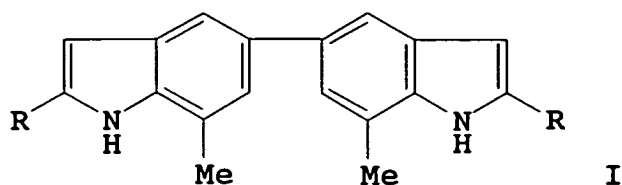


M



O
YIELD 28%

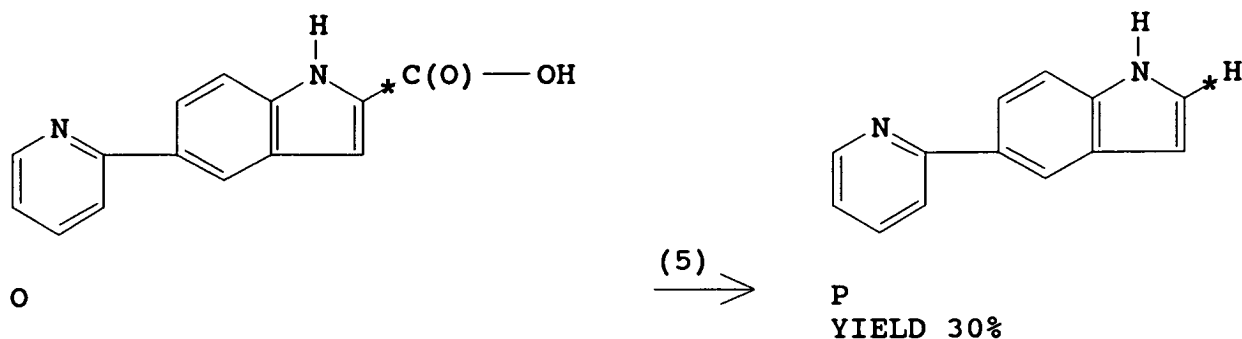
RX(5) RCT M 129450-58-4
PRO O 129431-59-0
NTE heat
AN 113:131932 CASREACT
TI Bisindoles. 28. Synthesis of 7,7'-dimethyl-5,5'-bis(1H-indole)
AU Zeghough, Djidel; Kadzhrishvili, D. O.; Samsoniya, Sh. A.; Suvorov, N. N.
CS Tbilisi. Gos. Univ., Tbilisi, 380028, USSR
SO Khim. Geterotsikl. Soedin. (1990), (3), 343-5
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
GI



AB Biindoledicarboxylate I (R = CO₂Et) was prepd. in 11% yield by cyclization of Et pyruvate 3,3'-dimethyl-4,4'-biphenylenehydrazone with polyphosphoric acid. Subsequent sapon. and thermal decarboxylation gave 28% I (R = H).

L5 ANSWER 5 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(5) OF 21 ...O ==> P



RX(5) RCT O 121217-70-7
PRO P 117908-10-8
NTE thermal

AN 111:23336 CASREACT

TI Indole derivatives. 133. Synthesis of 5-(2-pyridyl)indole

AU Akhvlediani, R. N.; Khachidze, M. M.; Eraksina, V. N.; Suvorov, N. N.

CS Mosk. Khim.-Tekhnol. Inst., Moscow, 125047, USSR

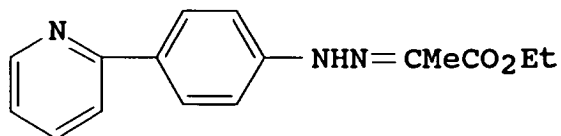
SO Khim. Geterotsikl. Soedin. (1988), (11), 1476-80

CODEN: KGSSAQ; ISSN: 0453-8234

DT Journal

LA Russian

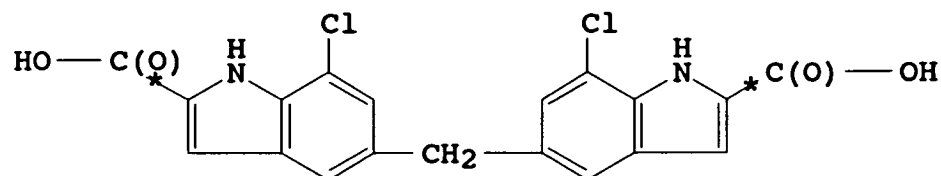
GI



AB Gomberg arylation of pyridine afforded 2-(4-nitrophenyl)pyridine, which was reduced with Fe shavings in aq. NH_4Cl to give hydrazone I. Japp-Klingemann indolization of I, followed by sapon. and thermal decarboxylation afforded 5-(2-pyridyl)indole.

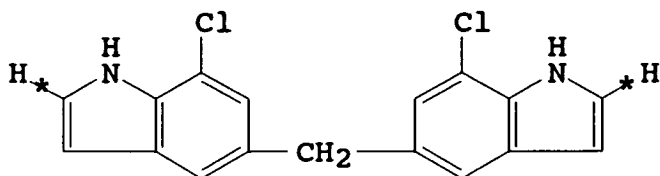
L5 ANSWER 6 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(3) OF 10 ...F ==> J



F

(3) >



J

YIELD 52%

RX(3) RCT F 120109-52-6
PRO J 120109-53-7
NTE Thermal

AN 110:173037 CASREACT

TI Bisindoles. 26. Synthesis of 7,7'-dichlorobis(5-indolyl)methane

AU Zeghugh, Dzh.; Kadzhrishvili, D. O.; Samsoniya, Sh. A.; Suvorov, N. N.; Kedelashvili, N. Z.

CS Tbilisi. Gos. Univ., Tbilisi, USSR

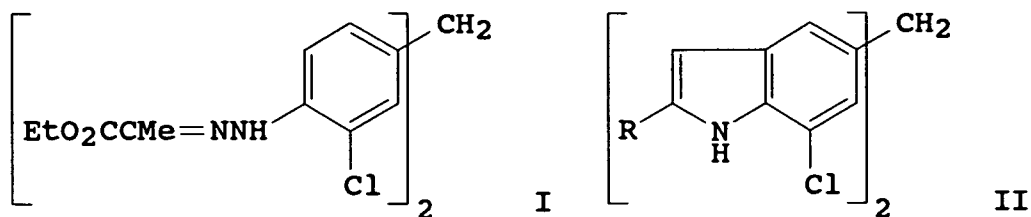
SO Khim. Geterotsikl. Soedin. (1988), (8), 1062-5

CODEN: KGSSAQ; ISSN: 0453-8234

DT Journal

LA Russian

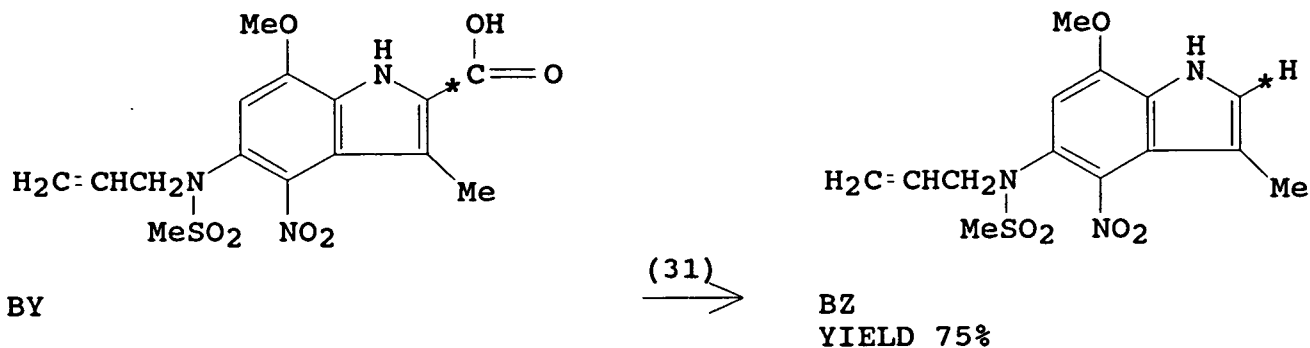
GI



AB Diphenylenemethane dihydrazone I underwent polyphosphoric Et ester-promoted cyclization to bis(carbethoxyindole)methane II (R = CO₂Et). The latter was saponified and thermally decarboxylated to give title compd. II (R = H). I was obtained as a mixt. of syn-syn, syn-anti, and anti-anti isomers from the corresponding dianiline deriv. by diazotization and condensation with Et pyruvate.

L5 ANSWER 7 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(31) OF 72 BY ==> BZ



RX(31) RCT BY 116911-59-2
RGT CA 1317-39-1 Cu₂O
PRO BZ 106994-17-6
SOL 127-19-5 AcNMe₂
NTE thermal

AN 109:190288 CASREACT

TI Synthesis of the left-hand ring of the antitumor antibiotic CC-1065 by an intramolecular carbenoid addition route. Synthesis and reactivity of 4-diazo-4,7-dihydroindol-7-ones and related compounds

AU Sundberg, Richard J.; Baxter, Ellen W.; Pitts, William J.; Ahmed-Schofield, Ruquia; Nishiguchi, Takeshi

CS Dep. Chem., Univ. Virginia, Charlottesville, VA, 22901, USA

SO J. Org. Chem. (1988), 53(21), 5097-107
CODEN: JOCEAH; ISSN: 0022-3263

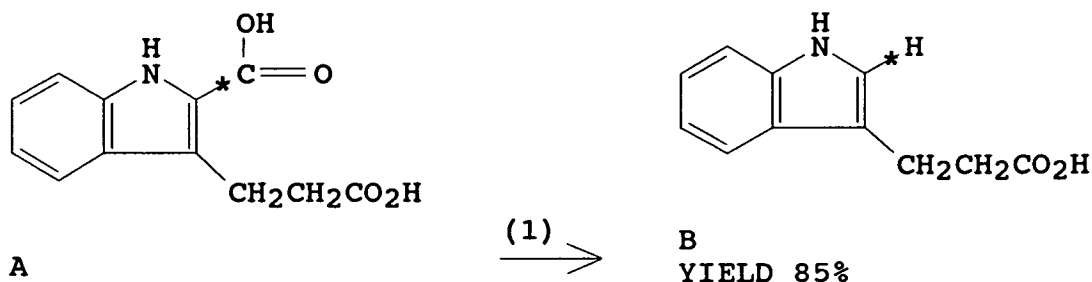
DT Journal
LA English
OS CJACS
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I (R = H, SO₂Ph; R₁ = SO₂Me; Z = N₂) were prepd. as potential precursors for the left-hand ring of antibiotic CC-1065 (II). Redn. and diazotization of (carbethoxyoxy)nitro(propenylsulfonyl)indole III, prepd. in 7 steps from 3,4-(PhCH₂O)(AcNH)C₆H₃NHSO₂Me (IV) gave I (R = H; R₁ = SO₂Me; Z = N₂). I (R = SO₂Ph; R₁ = SO₂Me; Z = N₂) was prepd. in 8 steps from IV analog a similar pathway. Photolysis, thermolysis, or transition metal-catalyzed decompn. of I (R₁ = SO₂Me, Z = N₂) gave mixts. of cyclopropanes V (by intramol. carbenoid addn.) and quinones I (R₁ = H, Z = O) (by O transfer from the SO₂ group).

L5 ANSWER 8 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(1) OF 21 ...A ==> B



RX(1) RCT A 31529-28-9
PRO B 830-96-6
NTE Thermal

AN 108:131499 CASREACT

TI Syntheses starting from 2-cyanocyclopentanone. Application of arylhydrazones of 5-cyano-5-oxopentanoic acid to the preparation of indole derivatives

AU Thi Anh Nga Trinh; Lamant, Maurice

CS Lab. Chim. Org., CNRS, Nantes, 44072, Fr.

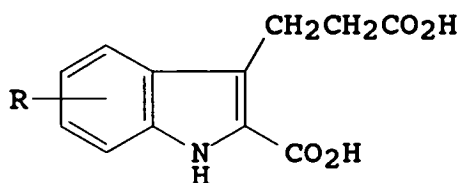
SO Bull. Soc. Chim. Fr. (1987), (2), 361-4

CODEN: BSCFAS; ISSN: 0037-8968

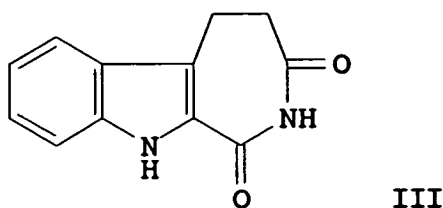
DT Journal

LA French

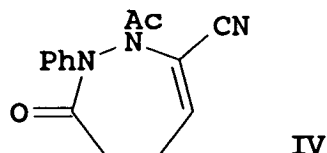
GI



II



III

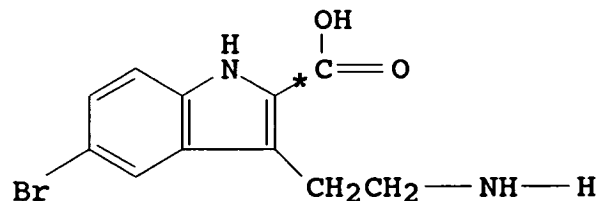


IV

AB Fischer's cyclization of (E)- and (Z)- $\text{RC}_6\text{H}_4\text{NHN:C(CN)(CH}_2)_3\text{CO}_2\text{H}$ (I; R = H, p-Me, p-Cl, p-Br, p-MeO, p-EtO, o-MeO) with HCl in EtOH affords (carboxyindolyl)propanoic acids (II) after sapon. of the intermediate amides. Treatment of I (R = p-Me, p-Cl) with ZnCl_2 in AcOH, however, gives azepino[3,4-b]indoles III. I (R = H) gives oxotetrahydrodiazepine IV upon treatment with polyphosphoric acid in AcOH.

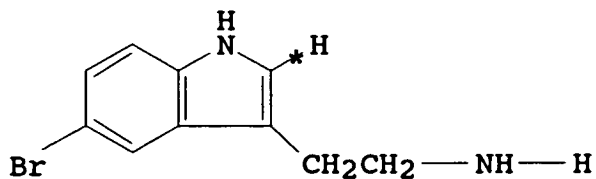
L5 ANSWER 9 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(3) OF 77 ...D ==> H...



D

(3) \longrightarrow



H
YIELD 58%

RX(3) RCT D 74058-58-5
RGT I 7664-93-9 H₂SO₄

PRO H 3610-42-2

SOL 7732-18-5 Water

AN 108:75693 CASREACT

TI Synthesis of Vinca alkaloids and related compounds. XXXIV. Synthesis of (3S,14S,16S)-bromovincamines and bromoapovincamines by regioselective bromination

AU Szabo, Lajos; Dobay, Laszlo; Kalasus, Gyorgy; Gacs-Baitz, Eszter; Tamas, Jozsef; Szantay, Csaba

CS Dep. Org. Chem., Tech. Univ., Budapest, H-1521, Hung.

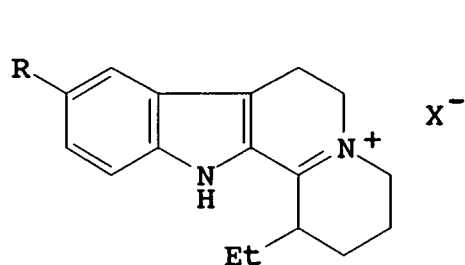
SO Arch. Pharm. (Weinheim, Ger.) (1987), 320(9), 781-9

CODEN: ARPMAS; ISSN: 0365-6233

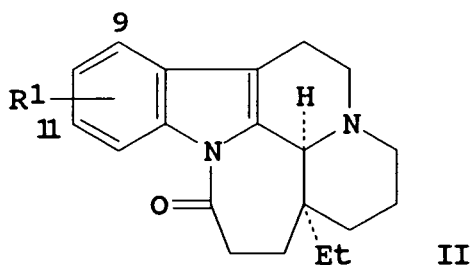
DT Journal

LA English

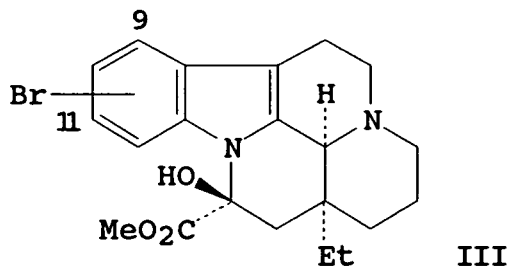
GI



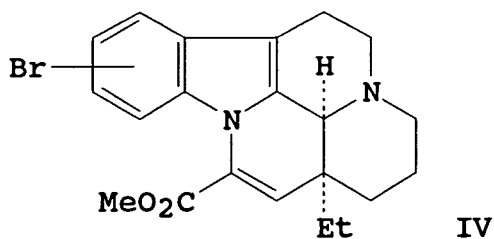
I



II



III



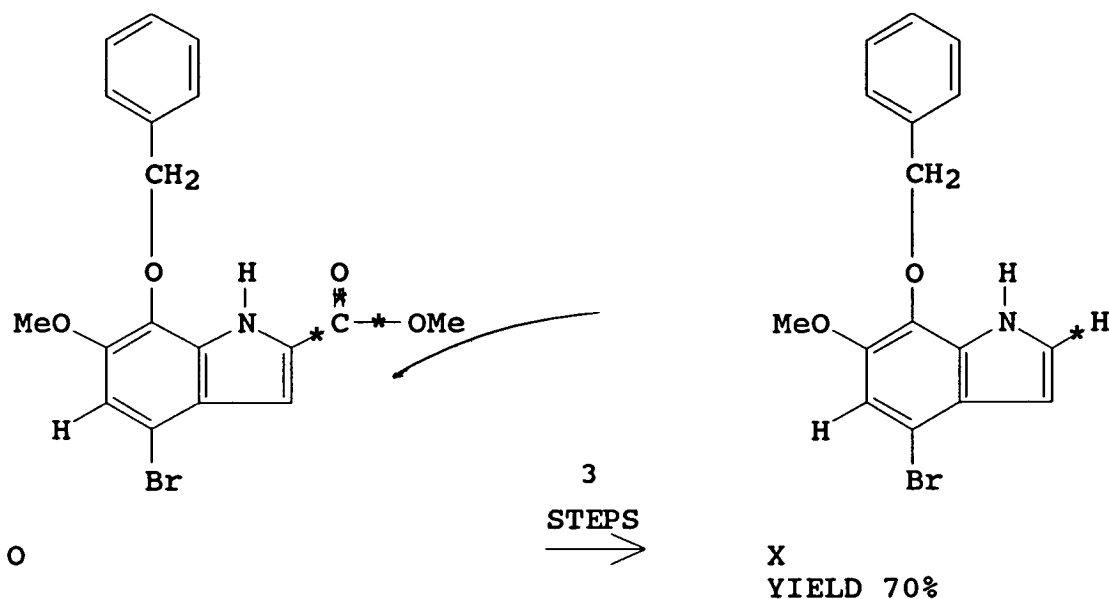
IV

AB Bromination of the iminium salt I (R = H, X = Cl) gave the 9-bromo deriv. I (R = Br, X = ClO4). Bromination of the lactam II (R1 = H) leads to a .apprx.7.5:1 mixt. of II (R1 = 11-Br, 9-Br). These precursors have been used to synthesize 9-, 10- and 11-bromovincamines III and 9-, 10- and 11-bromoapovincamines IV.

L5 ANSWER 10 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(42) OF 139 COMPOSED OF RX(5), RX(6), RX(8)

RX(42) O ==> X



RX(5) RCT O 102357-87-9
 RGT R 16853-85-3 LiAlH₄
 PRO Q 102357-88-0
 SOL 60-29-7 Et₂O

RX(6) RCT Q 102357-88-0
 RGT U 1313-13-9 MnO₂
 PRO T 102357-89-1
 SOL 75-09-2 CH₂Cl₂

RX(8) RCT T 102357-89-1
 PRO X 102357-90-4
 CAT 13938-94-8 Rhodium, carbonylchlorobis(triphenylphosphine)-
 , 6737-42-4 1,3-DPPP
 SOL 108-67-8 Mesitylene

AN 108:37451 CASREACT

TI Vinyl azides in heterocyclic synthesis. Part 8. Synthesis of the
 naturally occurring phosphodiesterase inhibitors PDE-I and PDE-II
 AU Bolton, Richard E.; Moody, Christopher J.; Rees, Charles W.; Tojo,
 Gabriel

CS Dep. Chem., Imp. Coll. Sci. Technol., London, SW7 2AY, UK

SO J. Chem. Soc., Perkin Trans. 1 (1987), (4), 931-5

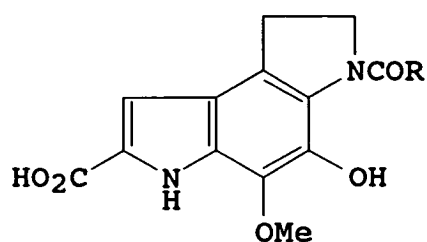
CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

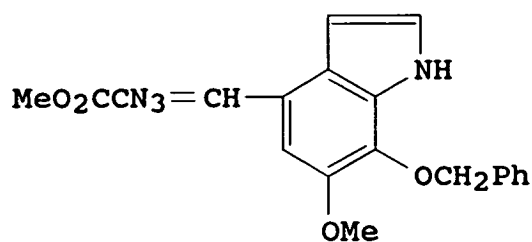
LA English

OS CJRSC

GI



I

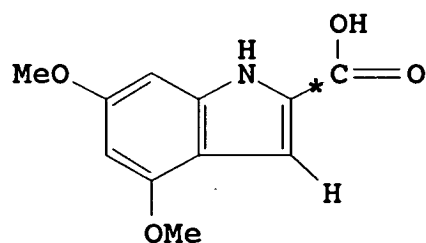


II

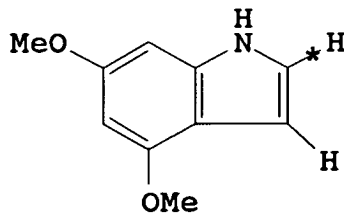
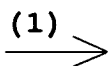
AB PDE-1 (I, R = NH₂) and PDE-II (I, R = Me) were prepd. from isovanillin. The route involves the construction of both pyrrole rings by vinylnitrene cyclizations, the key cyclization substrates being the azidoacrylates 2,4,5-Br(MeO)(PhCH₂O)C₆H₂CH:CN₃CO₂Me and II, prepd. from the aldehydes and N₃CH₂CO₂Me. The same tricyclic intermediate is converted into both PDE-I and PDE-II by selective redn., followed by carbamoylation or acetylation resp., and deprotection.

L5 ANSWER 11 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(1) OF 26 ...A ==> B

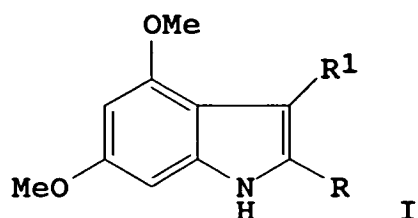


A



B

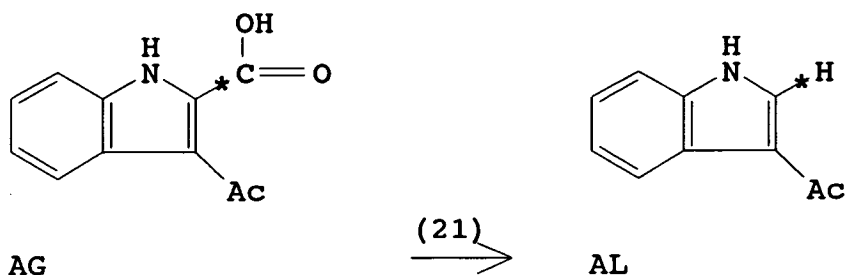
RX(1) RCT A 105776-11-2
 RGT C 7664-93-9 H₂SO₄
 PRO B 23659-87-2
 SOL 64-17-5 EtOH
 AN 106:18300 CASREACT
 TI Synthesis of 4,6-dimethoxyindoles
 AU Black, David S. C.; Kumar, Naresh; Wong, Laurence C. H.
 CS Sch. Chem., Univ. New South Wales, Kensington, 2033, Australia
 SO Aust. J. Chem. (1986), 39(1), 15-20
 CODEN: AJCHAS; ISSN: 0004-9425
 DT Journal
 LA English
 GI



AB Indoles I (R = H, R1 = H, Me, Ph; R = Me, R1 = H, Me; R = CO2Me, R1 = H, CO2Me; R = CO2H, R1 = H, CO2H, R = Ph, R1 = H, Ph; R = R1 = 2-pyridinyl) were prepd. by Bischler reaction followed by derivatization.

L5 ANSWER 12 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(21) OF 36 ...AG ==> AL



RX(21) RCT AG 105399-10-8
 PRO AL 703-80-0
 CAT 12017-79-7 Chromium copper oxide (CrCuO2)
 SOL 91-22-5 Quinoline

AN 105:226259 CASREACT

TI Synthetic studies on indoles and related compounds. XII. A simple general method for the C-3 acylation of ethyl indole-2-carboxylates

AU Murakami, Yasuoki; Tani, Masanobu; Suzuki, Michio; Sudoh, Keizo; Uesato, Midori; Tanaka, Kenjiro; Yokoyama, Yuusaku

CS Sch. Pharm. Sci., Toho Univ., Funabashi, 274, Japan

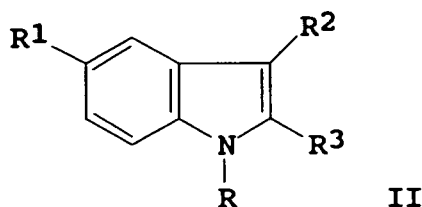
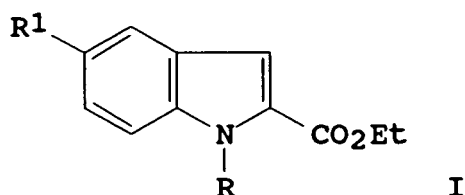
SO Chem. Pharm. Bull. (1985), 33(11), 4707-16

CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

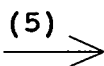
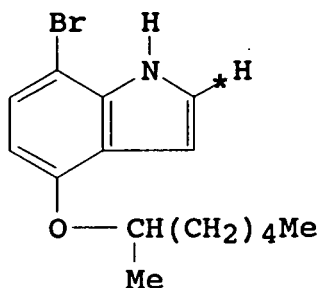
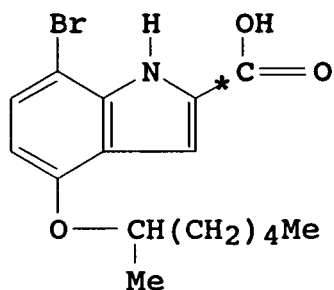
GI



AB Et indole-2-carboxylate I ($R = H, PhCH_2$; $R_1 = H, MeO, Cl$) were reacted with various carboxylic acids by using $(CF_3CO)_2O$ and H_3PO_4 (or polyphosphoric acid) to yield effectively Et 3-acylindole-2-carboxylates II ($R_2 = \text{e.g. Ac, Bz, Me}_3CCO, ClCH_2CO$; $R_3 = CO_2Et$). However, strongly acidic carboxylic acids and nitrogen-contg. carboxylic acids were poor acylating agents. Et 3-acylindole-2-carboxylates could easily be converted to 3-acylindoles.

L5 ANSWER 13 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(5) OF 45 ...M ==> Q...



RX(5) RCT M 102651-64-9
 PRO Q 102651-65-0
 CAT 11104-65-7 Chromium copper oxide
 SOL 91-22-5 Quinoline

AN 105:172225 CASREACT

TI Synthesis and analgesic evaluation of 4-(2-heptyloxy)-7-[(Z)-(3-hydroxycyclohexyl)]indole: a caveat on indole-phenol bioisosterism

AU Soll, Richard M.; Humber, Leslie G.; Deininger, David; Asselin, Andre A.; Chau, Thuy T.; Weichman, Barry M.

CS Chem. Pharmacol. Dep., Ayerst Lab. Res., Inc., Princeton, NJ, 08540, USA

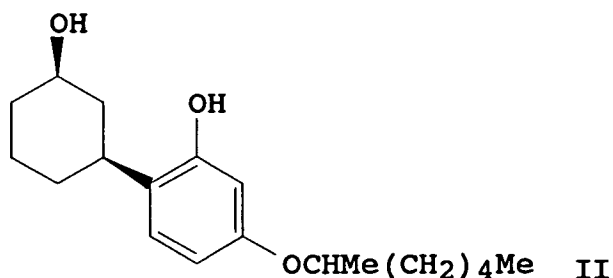
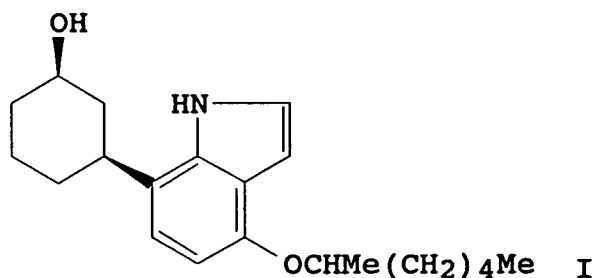
SO J. Med. Chem. (1986), 29(8), 1457-60

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

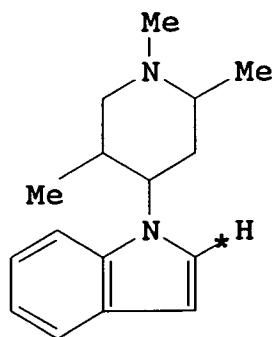
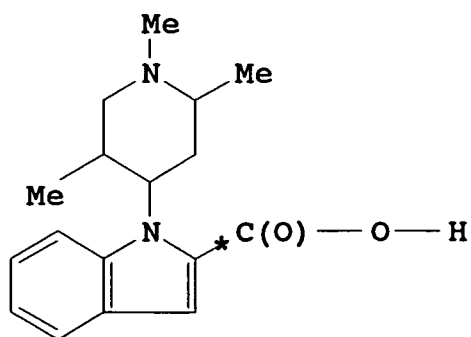
OS CJACS
GI



AB The indole I was prepd. as a bioisostere for the phenol II. I was obtained from 5,2-Br(HO)C₆H₃CHO via cyclization of 5,2-Br[Me(CH₂)₄CHMeO]C₆H₃CH:CN₃CO₂Me, decarboxylation of the resulting indole and reaction with cyclohexenone. In contrast, to II which had an ED₅₀ of 8.3 mg/kg, s.c. I was inactive in the phenylbenzoquinone writhing test. The absence of bioisosterism between the pyrrole ring and the phenolic OH group, in this instance, is discussed in terms of the circumstances that control the manifestation of bioisofunctionality between a pyrrole ring and a phenolic OH group, which functions as a H-bond donor.

L5 ANSWER 14 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(9) OF 43 ...R ==> S

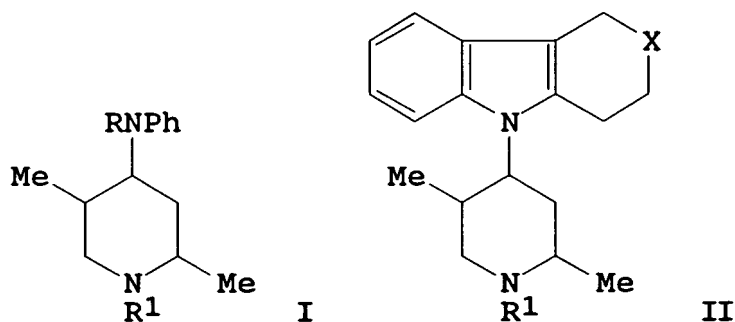


(9) \longrightarrow

R

S

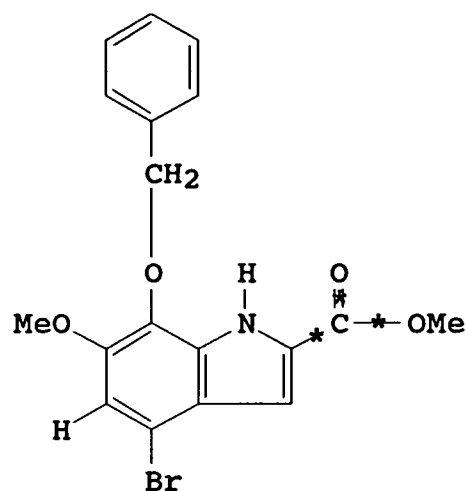
RX(9) RCT R 100907-63-9
PRO S 100907-66-2
NTE heat 205-210.degree.
AN 105:114874 CASREACT
TI Synthesis and heterocyclization of 1-phenyl-1-(1-alkyl-2,5-dimethyl-4-piperidyl)hydrazines
AU Vartanyan, R. S.; Martirosyan, V. O.; Kolozyan, K. R.; Vartanyan, S. A.
CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SO Arm. Khim. Zh. (1985), 38(5), 308-13
CODEN: AYKZAN; ISSN: 0515-9628
DT Journal
LA Russian
GI



AB Nitrosation of piperidines I ($R = H$, $R_1 = Me$, $PhCH_2$) by $NaNO_2$ in aq. HCl gave N-nitroso derivs. which were reduced by $LiAlH_4$ to give 72 and 82% hydrazines I ($R = NH_2$) which underwent a Fischer reaction with ketones to give 60-78% carbazoles and carbolines II ($R_1 = Me$, $PhCH_2$, $X = NMe$, NCH_2Ph , CH_2).

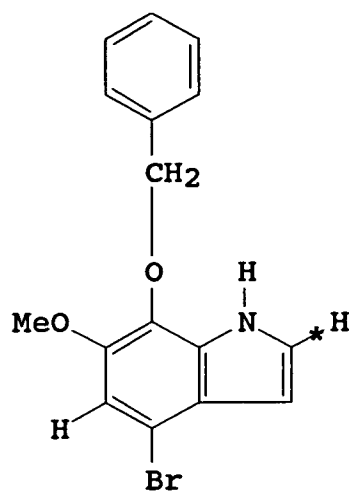
L5 ANSWER 15 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(25) OF 65 COMPOSED OF RX(3), RX(4), RX(5)
RX(25) F ==> N



F

3
STEPS
→



N

RX(3) RCT F 102357-87-9
RGT I 16853-85-3 LiAlH₄
PRO H 102357-88-0
SOL 60-29-7 Et₂O

RX(4) RCT H 102357-88-0
RGT L 1313-13-9 MnO₂
PRO K 102357-89-1
SOL 75-09-2 CH₂Cl₂

RX(5) RCT K 102357-89-1
PRO N 102357-90-4
CAT 13938-94-8 Rhodium, carbonylchlorobis(triphenylphosphine)-
, 6737-42-4 1,3-DPPP
SOL 108-67-8 Mesitylene

AN 104:224775 CASREACT

TI Synthesis of the phosphodiesterase inhibitors PDE-I and PDE-II

AU Bolton, Richard E.; Moody, Christopher J.; Rees, Charles W.; Tojo, Gabriel

CS Dep. Chem., Imp. Coll. Sci. Technol., London, SW7 2AY, UK

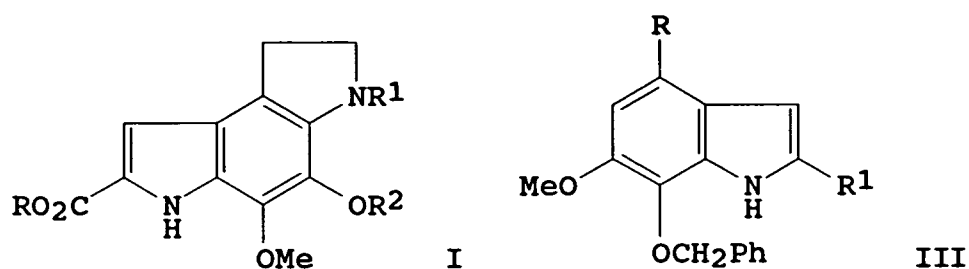
SO J. Chem. Soc., Chem. Commun. (1985), (24), 1775-6

CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

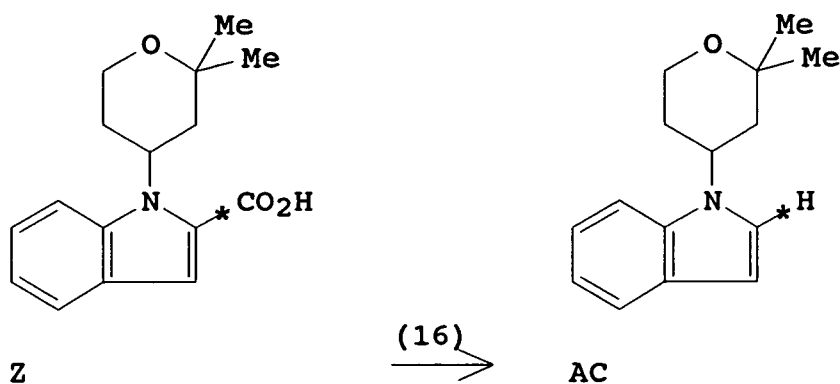
GI



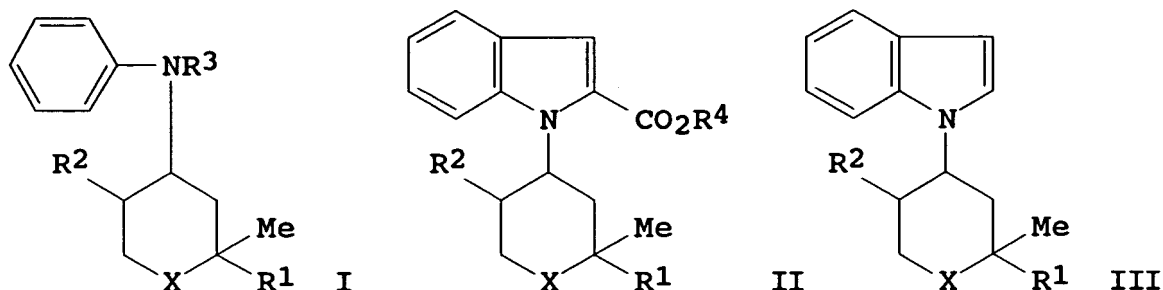
AB PDE-I and -II (I; R = R₂ = H, R₁ = CONH₂, Ac, resp.), which occur in *Streptomyces* MD769-C6, were prepd. from 5,4,2-RBr(MeO)C₆H₂OCH₂Ph (II; R = CHO) in 10 steps. The key steps were the cyclization of II (R = CH:CN₃CO₂Me) to the indole III (R = Br, R₁ = CO₂Me) and of the azide III (R = CH:CN₃CO₂Me, R₁ = H) to the pyrroloindole I (R = Me, R₁ = H, R₂ = CH₂Ph).

L5 ANSWER 16 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(16) OF 66 ...Z ==> AC



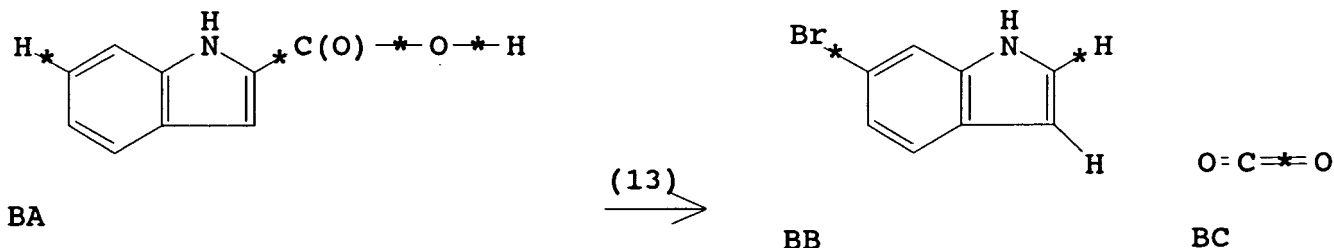
RX(16) RCT Z 100907-61-7
 PRO AC 100907-64-0
 NTE decarboxylation
 AN 104:129768 CASREACT
 TI New 1-substituted indoles
 AU Vartanyan, R. S.; Martirosyan, V. O.
 CS Inst. Tonkoi Org. Khim., Yerevan, USSR
 SO Arm. Khim. Zh. (1985), 38(7), 449-55
 CODEN: AYKZAN; ISSN: 0515-9628
 DT Journal
 LA Russian
 GI



AB Treating heterocycles I ($R_1 = \text{Me}, \text{H}$; $R_2 = \text{H}, \text{Me}$; $R_3 = \text{H}$; $X = \text{NMe}, \text{O}, \text{S}$) with NaNO_2 in concd. HCl gave intermediate nitroso compds. I ($R_3 = \text{NO}$), which were reduced with LiAlH_4 to give 80-84% amines I ($R_3 = \text{NH}_2$). Treating the latter with $\text{MeCOCOC}_2\text{Me}$ in MeOH or with $\text{MeCOCOC}_2\text{H}$ gave 71-79% hydrazones I ($R = \text{N:CMeCO}_2\text{Me}$) and 86-90% I ($R = \text{N:CMeCO}_2\text{H}$), resp. Cyclization of the hydrazones gave 73-79% indoles II ($R_4 = \text{Me}$), which were saponified to give 70-84% II ($R_4 = \text{H}$). Decarboxylation of the latter at 205-210.degree. gave 61-78% indoles III.

L5 ANSWER 17 OF 17 CASREACT COPYRIGHT 1994 ACS

RX(13) OF 263 BA ==> BB + BC...



RX(13) RCT BA 1477-50-5
RGT AX 7440-50-8 Cu, AY 91-22-5 Quinoline
PRO BB 52415-29-9, BC 124-38-9

AN 103:71643 CASREACT

TI Amino acids and peptides, XLVIII. Total synthesis and biomimetic formation of clionamide derivatives

AU Schmidt, Ulrich; Lieberknecht, Albrecht; Griesser, Helmut; Boekens, Hilmar

CS Inst. Org. Chem., Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.

SO Liebigs Ann. Chem. (1985), (4), 785-93

CODEN: LACHDL; ISSN: 0170-2041

DT Journal

LA German

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The total synthesis of tetraacetylclionamide I from amine II and (S)-tryptophan III (Boc = Me₃CO₂C) is described. Thus, II was condensed with III to give amide IV (RR₁ = O), which was reduced by NaCNBH₃ to give a diastereoisomeric mixt. of IV (R = H, R₁ = OH), which was converted to the (E)-enamide via a selenium oxide elimination reaction. II and III were prepd. by std. methods. The biomimetic prepn. of debromoclionamide deriv. V by decarboxylation of the corresponding dehydro amino acid deriv. is described.

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FILE 'CASREACT' ENTERED AT 09:12:15 ON 15 NOV 94

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L3	29 S L1 FUL
L4	STR L1
L5	17 SEARC SSS FUL L4 SUB=L3

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